

$\Delta T$  dependencies [3] need to be fitted by least squares minimization. JANA2006 has recently with success implemented this new approach to rigorously refine these parameters for calibration purpose. This presentation will compare the approach between JANA2006, Fullprof [4] and also GSAS.

In the second part of the presentation we will discuss the advantage of the new approach using magnetic superspace groups introduced into the JANA2006 software. Such tool is adequate with high resolution data which highlights more complex magnetic ordering.

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**Keywords:** software, time-of-flight, neutron

## MS.69.4

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### Fitting a square peg into a round hole: Simulating a modulated protein crystal

Jeffrey J. Lovelace,<sup>a</sup> Vaclav Petricek,<sup>b</sup> Michal Dusek,<sup>b</sup> Sander van Smaalen,<sup>c</sup> Garib N. Murshudov,<sup>d</sup> Gloria E. O. Borgstahl,<sup>a</sup> <sup>a</sup>*Eppley Institute for Cancer Research and Allied Diseases, 987696 Nebraska Medical Center, Omaha, NE 68198, (USA)*. <sup>b</sup>*Institute of Physics, Academy of Sciences of the Czech Republic, Praha, (Czech Republic)*. <sup>c</sup>*Laboratory of Crystallography, University of Bayreuth, 95440 Bayreuth, (Germany)*. <sup>d</sup>*YSBL, Chemistry Department, University of York, (York), YO10 5DD (UK)*. E-mail: gborgstahl@unmc.edu

We are interested in solving a protein crystal structure that contains an incommensurate modulation in one direction, a so-called (3+1) dimensional modulation. Several roadblocks in this structure determination have been found and will be solved by simulating this type of crystal and diffraction data. In the world of small molecules, modulated datasets are handled in a routine fashion. The existing software supplied with most X-ray systems can index the satellite reflections with the associated q-vectors, predict, integrate and scale the data. Then the Jana software suite can refine and solve the modulated small molecule structure. The resulting data can be neatly stored into a CIF file and submitted for archival and publication.

For protein crystallography it is an entirely different situation. Great strides have been made in processing modulated macromolecular diffraction data. Most protein data processing software cannot handle satellite reflections but the recently released EVAL15 software can process incommensurately modulated data for both protein and small molecules. Then SADABS can be purchased as standalone software to scale the resulting indexed and integrated values from EVAL15 producing an HK6 file. The HK6 format contains up to 6 indices (HKL + 3 q-vectors). It is at this point that there is currently no pathway for solving an incommensurately modulated protein crystal. Incommensurate protein models cannot be fit to 4D electron density maps, these structures cannot be refined against the modulated diffraction data and even if they could it would not be possible to store the structure in existing mmCIF or PDB formats. Thus significant modifications of existing tools are required to enable the solution of the first incommensurately modulated protein structure.

As a first step we are in the process of creating a (3+1)D training set that can be used to test approaches for modeling and refining a modulated protein structure against the corresponding diffraction data. The procedure to create the training dataset is backwards from normal data processing. First a modulated structure is generated and then the

resulting main and satellite reflections are simulated. The reflections are represented in (3+1)D indexing. Then everything needs is written into a CIF-type format that can be read in and used by protein crystallographic software. The problems we have encountered as well as the solutions we have selected will be presented and evaluated. The overall result was that each step of the process was much more challenging than we had initially envisioned.

**Keywords:** modulation, CIF, simulation, incommensurate

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### Higher-dimensional crystallography of n-fold quasiperiodic tilings (n=7-15)

Sofia Deloudi, Walter Steurer, *Laboratory of Crystallography, Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse 10, 8093 Zurich, (Switzerland)*. E-mail: deloudi@mat.ethz.ch

The study of periodic average structures gives periodic lattices which closely correspond to the quasiperiodic tilings. This concept is of particular interest for the study of geometrical aspects of quasicrystal-to-crystal phase transformations [1], formation and understanding of quasicrystal-crystal interfaces [2], as well as the intrinsic band-gap behavior of phononic or photonic quasicrystals [3], [4]. For a general overview, see e.g. [5]. A detailed discussion on the periodic average structures of the Penrose and Ammann tiling (pentagonal, resp. icosahedral symmetry), as well as the Fibonacci sequence, can be found in [6].

We studied two-dimensional quasiperiodic tilings with heptagonal, octagonal, enneagonal, decagonal, hendecagonal, dodecagonal, triskaidecagonal and pentakaidecagonal symmetry with regard to their periodic average structures. By identifying the best (most representative) periodic average structures for each case, we have found that quasiperiodic tilings with different symmetries can show significantly different degrees of average periodicity.

The complexity of the periodic average structures and the degree of average periodicity depend on the minimum dimensionality and topological constitution of the hypersurfaces. The distribution of deviations from periodicity is given by the projected volume function of the higher-dimensional hypersurfaces upon physical space. The octagonal, decagonal and dodecagonal tilings show the smallest deviation from their periodic average structures. They have two-dimensional hypersurfaces, and the distribution of deviations can be described by simple sep-functions.

In the 7-, 9-, 11-, 13- and 15-fold tilings, the dimensionality of the hypersurfaces is greater than two, and is therefore reduced in the projection upon a two-dimensional space. This results in a non-homogeneous distribution of deviations from the periodic average lattice, and therefore in a higher complexity of the periodic average structures. But while the 7- and 9-fold tilings can still be described reasonably by at least one periodic average structure, the 11-, 13-, and 15-fold cases show a very low degree of average periodicity. A representation of the infinite tilings by their periodic average structures is generally unfavorable for systems of such high dimensionality. The concept of a periodic average structure can here best be used on finite systems like in photonic and phononic quasiperiodic crystals. The infinite systems on the other hand, show deviations from the periodic lattice that densely fill the unit cell of the later. However, the distribution of deviations is highly inhomogeneous. The study of periodic average structures gives therefore still information about which periodic lattices match the quasiperiodic ones best.

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